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CO_2 capture technical analysis for gas turbine flue gases with complementary cycle assistance including non linear mathematical modeling

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Abstract

In this study, a *Gas Turbine (GT)* fed by the fossil fuel of type PG6561B (installed at South-Pars Gas Field) is simulated and implemented as an integrated model in *Cycle-Tempo* and *GasTurb-11*. Next, the energy driving forces, which cause of the temperature difference between the GT flue gases and the input stream to CO_2 capture cycle, are applied in the *Heat Recovery Steam Generator (HRSG)*. This process is also designed and modeled in *Cycle-Tempo.* Then, the local power plant data acquisition is done based on the data loggers, which are applied as the initial values for the modeling evaluation purposes. Finally, based on the CO_2 abatement and emission control, the post-combustion CO_2 capture cycle is simulated in *MATLAB* using the method of lines discretization in the spatial direction along the length of the columns.

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Keywords*: CO_2 Capture; Integrated Comprehensive Cycle; Gas Turbine; HRSG; Dynamic Simulation.*

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Nomenclature

LHV	Lower Heating Value, *(Kj/kg)*
C_i^l	Concentration of component in liquid phase, *(mol/m^3)*
T	Time, *(s)*
U	Velocity of fluid, *(m/s)*
H	Height, *(m)*
$\dot{n}_{i,d}$	Component diffusion mole flow, *(mol/m^{3}s)*
$R_{i,gen}$	Component mole generation value, *(mol/m^{3}s)*
C_i^v	Concentration of component in vapor phase, *(mol/m^3)*
T^l	Temperature of liquid inside control volume, *(k)*
$\Delta\tilde{H}_i^{vl}$	Difference between the enthalpy of vapor and liquid for each species, *(J/mol)*
$\tilde{C}p_i^l$	Specific molar heat capacity of species in liquid phase, *(J/mol K)*
ΔH_{RE}	Enthalpy of reaction, *(J/mol)*
U_{lv}	Overall Convective heat transfer coefficient, *(J/m^2 K S)*
T^v	Temperature of liquid inside control volume, *(k)*
$\tilde{C}p_i^v$	Concentration of component in vapor phase, *(mol/m^3)*

Acronyms

HRSG	Heat Recovery Steam Generation
GT	Gas Turbine
MEA	Monoethanolamine

1. Introduction

The increasing rate of carbon dioxide is approximately estimated at 1.5ppmv per year, which corresponds to a temperature increase in the range of 4 to 8 degrees in the coming century. As it was reported in 2000, 23.5 giga-tonnes of CO_2 were released from man-made resources with a 60% share discharged from the point sources such as fossil fuel power stations, industrial processes, and oil and gas extraction plants [1].

Several investigations in CO_2 capture have been done in power-plants industry since then. These investigations mainly focus on coal-fired cycles, and CO_2 capture systems are considered individually. In this paper, we consider different stages of the process, which include power and HRSG cycles and CO_2 capture system. In particular, we apply the studied case of the GT– 42 MW type PG6561B for modeling and CO_2 capture purpose.

Generally, water and CO_2 are the main products of fossil fuels combustions. The emission of carbon dioxide has specific effects on increasing the amounts of greenhouse gases, and consequently causes the climate changes and global warning, which is considered as a worldwide challenge [2]. In this respect, some international rules have been legislated in order to reduce CO_2 emissions to the atmosphere. As a result, the CO_2 capture systems have got so much attention recently and have been improved to meet some controlling criterions [3].

CO_2 capture consists of three different types in technology reviews, namely, Post-combustion, Pre-combustion and Oxy-fuel. Among these methods, we mainly apply the post-combustion chemical absorption with RNH_2 or MEA (Monoethanolamine) solution, which is the most common and precisely developed technology to capture CO_2 from combustion-based power plants [4], and is quantified to 97.70% in consistency of CO_2 removal in the flue gas inlet. The rate of this value is equal to 7.3640Kg/s, which is appropriate at 7.59176 Kg/s inlet. By these means, the global model target is achieved.

2. System Approach

The approach of this study can be categorized as the following:

- The quantification of the amount of carbon dioxide coming out of the natural gas combustion in GT in various atmospheric conditions i.e. summer and winter cases with different humidity and temperature profiles.
- Applying the hot flue gases as an energy driving force due to combustion, in HRSG for the heat recovery purposes.
- The dynamic simulation of CO_2 capture cycle, time intervals process analysis based on molecular dynamics and reactions to achieve CO_2 removal percentage target (Above 95%).

3. System Configuration

As it is illustrated in figure 1, this system is comprised of different sections. In this work, 42MW GT is applied to enter compressed air, which burns at a combustion chamber with natural gas. The out-coming hot flue gases run the turbine, which is coupled with the generator that produces power [5]. After this stage, recoverable energy which belongs to the flue gases is applied in HRSG cycle and as a consequence, the 530°C super-heated steam is also produced. Before the flue gases enter the absorption column, it is necessary to cool down and compress the gases to meet the absorber operational conditions. The absorption tower, which is a large cylindrical tower, is filled with the packing and operates within a temperature range of 40-45ºC. The inlet gas is entered at the bottom of the tower and flows up through

the tower while the lean liquid mixture (30% MEA and 70% water) is rinsed at the top and showers down over the packing [6]. The rich amine is pumped up from the bottom of the absorption tower to the heat-exchanger and top of the stripping tower. The purpose of the stripper is heating up the mixture to 110-120°C temperature level to pursue reverse chemical reactions and to decrease the solubility of CO_2 in the solution [7].

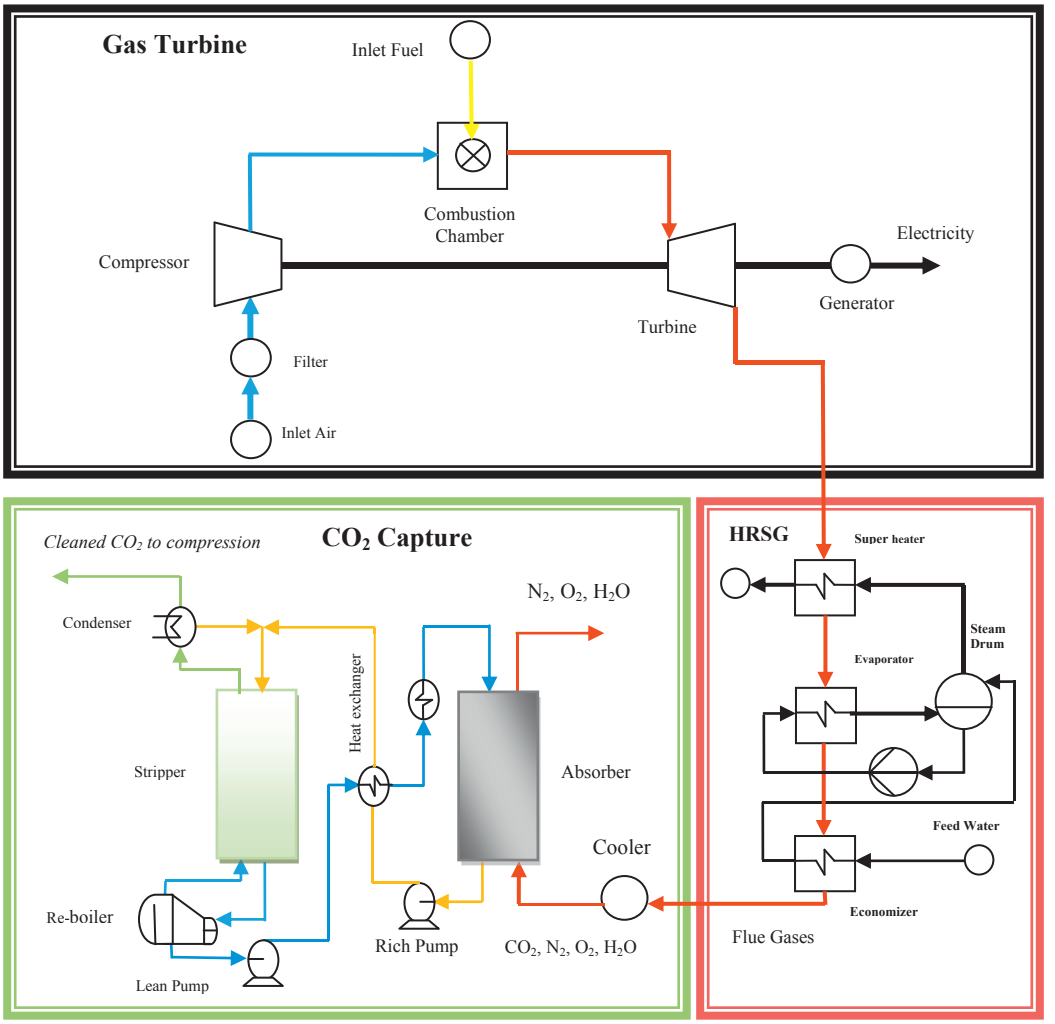


Fig. 1. Schematic of comprehensive cycle includes GT, HRSG and Amine based CO_2 capture system

4. System Modeling

4.1. GT and HRSG Modeling

GT and HRSG models have been built in Cycle-Tempo Software [8]. The main purpose of using this software was to create a model in the steady state. Based on the site reports, the main input assumptions of the model can be characterized as following the tables 1 and 2.

Table 1. GT modeling input data

No	Input	Unit	Value			
1	**Inlet Air**					
1-1	Temperature	°c	5	37	43	48
1-2	Relative humidity	%	100	65	65	65
1-3	Pressure	Bar	0.0997			
1-4	Mass flow	Kg/s	145.253			
1-5	Pressure drop in air filter	Bar	0.01			
2	**Compressor**					
2-1	Output pressure	Bar	11.6474			
2-2	Isentropic efficiency		0.8533			
3	**Inlet Fuel and Combustion Chamber**					
3-1	Inlet fuel temperature	°c	15			
3-2	Inlet fuel pressure	Bar	25.2			
3-3	LHV	Kj/Kg	45661			
3-4	Output pressure	Bar	11.056			
4	**Turbine**					
4-1	Isentropic efficiency		0.8			

Table 2. HRSG modeling input data

No	Input	Unit	Value
1	**Super-heater**		
1-1	Output steam temperature	°c	530
1-2	Flue gases pressure drop	Bar	1
1-3	Steam pressure drop	Bar	0.01
2	**Evaporator**		
2-1	Flue gases pressure drop	Bar	1.5
2-2	Steam pressure drop	Bar	0.1
2-3	ΔT_{Steam}	°c	10
3	**Economizer**		
3-1	Flue gases pressure drop	Bar	1
3-2	Water pressure drop	Bar	0.1
3-3	ΔT_{Water}	°c	15
4	**Feed water**		
4-1	Temperature	°c	41
4-2	Pressure	Bar	25
5	**Pump**		
5-1	Isentropic efficiency		0.75
6	**Drum**		
6-1	$\frac{Steam}{Water}$		4

It should be noted that the other characteristics which are necessary to design point's simulation are extracted from the mentioned site reports. In addition, for any further steps in the simulations, we need to define the exact properties of the natural gas.

4.2. Dynamic Simulation Proposed CO_2 Capture System Modeling

The simulation of the system is implemented in MATLAB using the method of discreteness in the spatial direction along the length of the absorber and stripper columns. The system is characterized by the closed loop recirculation of the Monoethanolamine Solution (RNH_2). Numerical solver ODE15s-(solution method) is applied to solve the model including time durations (Dynamic simulation approach). This integrated comprehensive cycle needs to be processed for one hour to pass the transient state and reach the steady state of the carbon dioxide capture dominated value.

4.2.1. Reactions

The following chemical reactions are taking place simultaneously in the CO_2 abatement cycle [9]:

1. Overall reaction rate of MEA and Carbon dioxide
$$2MEA + CO_2 \leftrightarrow MEACOO^- + MEAH^+$$
2. Hydrolyze of CO_2 with Water
$$CO_2 + 2H_2O \leftrightarrow HCO_3^- + H_3O^+$$
3. Bicarbonate Formation
$$CO_2 + OH^- \leftrightarrow HCO_3^-$$
4. Disassociation of Water
$$2H_2O \leftrightarrow H_3O^+ + OH^-$$
5. Dissociation of MEA^+
$$MEA^+ + H_2O \leftrightarrow MEA + H_3O^+$$
6. MEA Carbonate
$$H_2O + MEACOO^- \leftrightarrow HCO_3^- + MEA$$

4.2.2. Equations

The chemical reactions of MEA and CO_2 are included in the model, and Henry's law describes the vapor-liquid equilibrium for CO_2 [10, 11]. The concentrations of MEA, H_2O, N_2 and O_2 in both phases are calculated according to Peng-Robinson equation of state [12], using the fugacity of individual species [13]. The main equations to determine the concentrations and temperatures of liquid and gas phases are listed below [14]:

$$\frac{dc_i^l}{dt} = u\frac{dc_i^l}{dz} - \dot{n}_{i,d} + R_{i,gen} \quad (1)$$

$$\frac{dc_i^v}{dt} = -u\frac{dc_i^v}{dz} + \dot{n}_{i,d} \quad (2)$$

$$\frac{dT^l}{dt} = -u\frac{dT^l}{dz} - \frac{[\dot{n}_d]^T[\Delta\tilde{H}_i^{vl}]}{[C_i^l]^T[\tilde{C}p_i^l]} - \frac{\dot{n}_{CO2}\,\Delta H_{RE}}{[C_i^l]^T[\tilde{C}p_i^l]} - \frac{U_{T,lv}(T^l - T^v)}{[C_i^l]^T[\tilde{C}p_i^l]} \quad (3)$$

$$\frac{dT^v}{dt} = -u\frac{dT^v}{dz} - \frac{[\dot{n}_d]^T[\Delta\tilde{H}_i^{vl}]}{[C_i^v]^T[\tilde{C}p_i^v]} + \frac{U_{T,lv}(T^l - T^v)}{[C_i^v]^T[\tilde{C}p_i^v]} \quad (4)$$

4.2.3. Assumptions

Table 3 lists the main input assumptions of the model.

Table 3. CO_2 capture system Input data

No	Input	Unit	Value
1	Mole flow of CO_2 into the capture system	Mol/s	172.54
2	Absorber gas inlet temperature	K	313
3	Volume flow of liquid	M^3/s	0.67875
4	Condenser reflux percentage	%	10
5	Re-boiler pressure	Pa	200000
6	Re-boiler temperature	K	394.2
7	Absorber liquid temperature	K	318
8	Condenser liquid temperature	K	380
9	Lean pump pressure	m	15
10	Rich pump pressure	m	15

5. Results and Conclusions

Gas Turbine and HRSG modeling results indicate the percentage of carbon dioxide variations in the flue gases, which is between 3.18% and 3.32%. The amount of carbon dioxide has minor changes under different conditions of GT operations. These results, which have been also verified with GT modeling in Gas-Turb11 software, are shown in Table4:

Table 4. GT and HRSG modeling results

No	Inlet air temperature (^oC)	CO_2 percentage in flue gases (%)	Power generation (MW)	Net Efficiency (%)	Turbine flue gases temperature (^oC)	Flue gases mass flow (Kg/s)
1	5	3.32	42.74	31.69	555	148.20
2	37	3.21	34.91	29.75	578	129.23
3	43	3.18	33.38	29.10	583	125.33
4	48	3.32	32.11	27.01	587	122.19

According to table 3, as the inlet air temperature increases, the GT power generation as well as the flue gases mass flow will decrease, and the flue gases temperature increases. On the other hand, since the percentage of CO_2 varies in the flue gases, sensitivity analysis under the various conditions of ambient temperature is not considered, and 5^{oC} is applied as the inlet air temperature for dynamic simulation of the absorption cycle. In this case, the flue gases mole flow is 28.52 Kg/kmol that 3.32% of it includes CO_2, which produces 179560 tonnes of CO_2 annual.

Four scenarios with different absorbers and stripper heights and diameters are applied in CO_2 capture system simulations. These results are shown in the table 5, as the following:

Table 5. CO_2 capture system simulation results

No	Absorber height (m)	Absorber diameter (m)	Stripper height (m)	Stripper diameter (m)	CO_2 capture percentage (%)
1	10	2.75	5	1.5	35.32
2	15	2.75	10	1.5	53.48
3	15	10.00	8	3.0	97.70
4	15	10.00	10	5.0	97.70

Based on the aforementioned results, even though CO_2 capture percentage in the first and second runs do not agree, even with the excepted range, it is improved to 97.70% in the third run. Consequently, the values of 15m and 10m are respectively accepted for the height and the diameter of the absorber. Similarly, to obtain the desirable CO_2 recovery, a stripper with 10m height and 5m diameter is considered. The process of achieving these values using *MATLAB* is shown through figures 2-8.

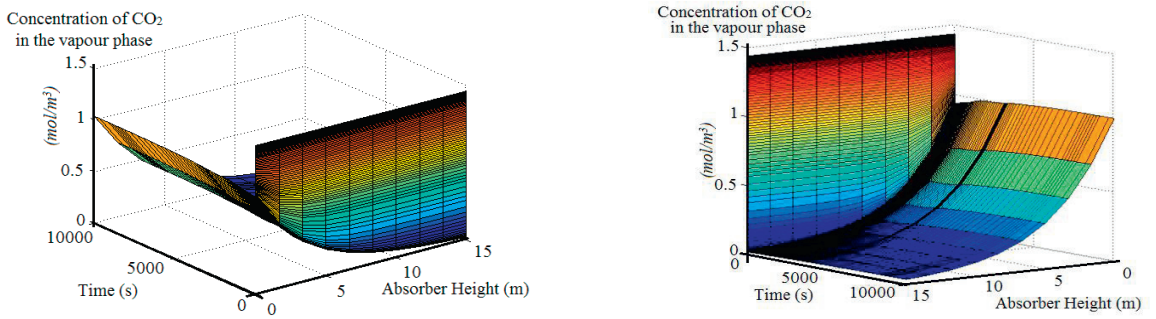


Fig. 2. Concentration of CO_2 in the vapour phase for the absorber *(mol/m³)*

Figure 2 plots CO_2 concentration in the absorption column and expresses that CO_2 is captured from when it enters at the bottom of the absorber until the point it leaves at the top. The removal percentage is estimated at 97.70%, which is within the range that is expected according to the global model target. The removal rate is the greatest at the bottom of the tower and, as the concentration in the gas tends to zero emission, it decreases. The height of the tower has a noticeable effect on CO_2 capture.

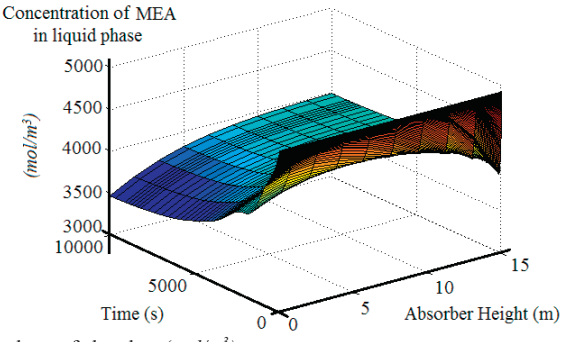


Fig. 3. Concentration of MEA in liquid phase of absorber *(mol/m³)*

Figure 3 plots of the concentration of MEA in the liquid phase of the absorber. The plot shows a smooth curve as the MEA is consumed while it slowly decreased the tower from the inlet at the top.

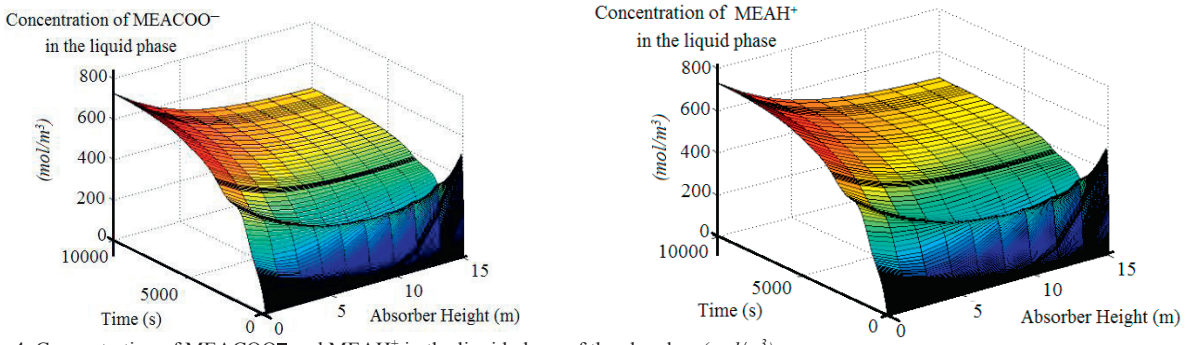


Fig. 4. Concentration of $MEACOO^-$ and $MEAH^+$ in the liquid phase of the absorber *(mol/m³)*

The concentration of $MEACOO^-$ in the absorber liquid phase is shown in figure 4. The rendered code indicates the opposite trend to that of MEA, i.e. $MEACOO^-$ is produced as the liquid which travels down the column

absorbing CO_2. $MEAH^+$ concentration plot has the same shape and values as $MEACOO^-$, and the level of increase is about 0.5 times greater than the consumption rate of the MEA because in the operating range of the tower, two moles of MEA is required to remove one mole of CO_2.

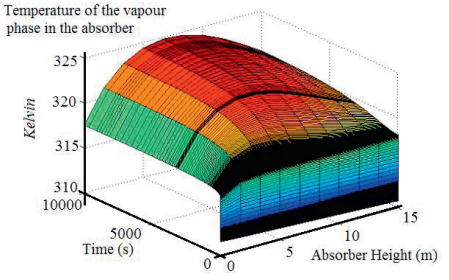


Fig. 5. Temperature of the vapour phase in the absorber *(k)*

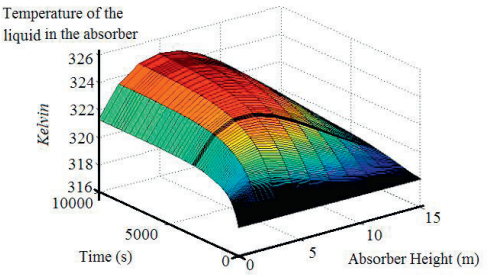


Fig. 6. Temperature of the liquid in the absorber *(k)*

Figure 5 shows the vapor phase temperature profile that follows almost the same manners as the liquid temperature profile. At the bottom of the tower, the gas phase receives heat from the liquid phase and then at the top of the tower, the gas phase transfers heat to the liquid phase.

Figure 6 is the plot of the liquid temperature profile. It can be characterized as an increase to its maximum value in about 1/3 of the way down the tower and then a decrease. The increase is a consequence of the heat supplied from the exothermic reaction between MEA and CO_2.

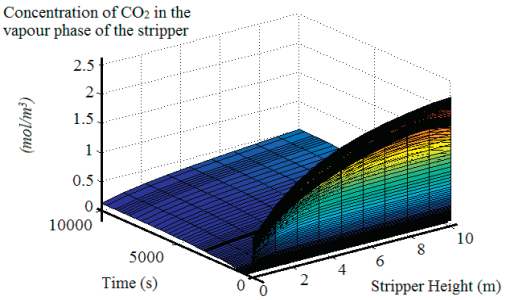
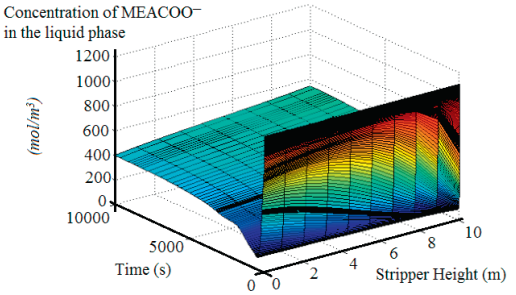


Fig. 7. Concentration of CO_2 in the vapour phase of the stripper *(mol/m^3)*

The CO_2 concentration in the cleaned gas at the stripper is shown in figure 7. The concentration increases quickly as the reaction spruced rapidly at the bottom of the tower where the steam enters the tower to supply the energy.



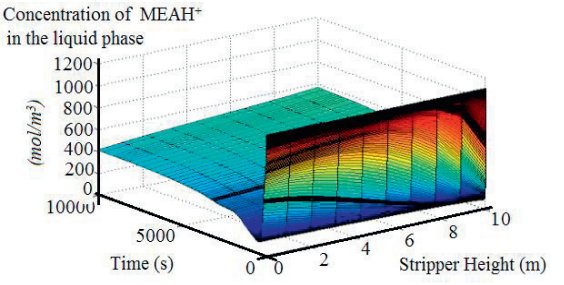


Fig. 8. Concentration of $MEACOO^-$ and $MEAH^+$ in the liquid phase of the stripper *(mol/m^3)*

The reversibility of the chemical reactions is indicated in figure 8. As shown above, $MEAH^+$ concentration is decreasing as the liquid enters the stripper. The concentration of the $MEACOO^-$ ion has the same profile.

In short, the major conclusions headlines can be listed as below:

- The modeling of the CO_2 capture system is a complex problem with many interactions. In this model, many assumptions and simplifications have been made while the results are still reasonable and in acceptable range.
- A Henry's law for CO_2 as a function of temperature, solubility of CO_2 in water, solubility of CO_2 in MEA and ionic strength is adequate to describe the vapor-liquid equilibrium for Carbon dioxide.
- The residence time of the liquids in the absorption tower has a great effect on the result. Thus increasing the absorption tower diameter and height produces a higher removal rate.
- There are many parameters and inputs that can affect the results, so finding an optimal solution is a challenging task, especially if we include the balance between capital and operational costs.
- Significant amounts of H_2O and MEA leave the system with the exhaust gas and the purified steam. Therefore, water wash and make up water and MEA should be applied.

6. Recommendations for future work

In future work, the optimization of MEA-based capture process integrated with power plants will be examined. The MEA-based capture process needs to be optimized for the operation, as well.

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